

Geometric spectral inversion for singular potentials

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The function $E = F(v)$ expresses the dependence of a discrete eigenvalue E of the Schrödinger Hamiltonian $H = -\Delta + vf(r)$ on the coupling parameter v . We use envelope theory to generate a functional sequence $\{f^{[k]}(r)\}$ to reconstruct $f(r)$ from $F(v)$ starting from a seed potential $f^{[0]}(r)$. In the power-law or log cases the inversion can be effected analytically and is complete in just two steps. In other cases convergence is observed numerically. To provide concrete illustrations of the inversion method it is first applied to the Hulthén potential, and it is then used to invert spectral data generated by singular potentials with shapes of the form $f(r) = -a/r + b \operatorname{sgn}(q)r^q$ and $f(r) = -a/r + b \ln(r)$, $a, b > 0$. For the class of attractive central potentials with shapes $f(r) = g(r)/r$, with $g(0) < 0$ and $g'(r) \geq 0$, we prove that the ground-state energy curve $F(v)$ determines $f(r)$ uniquely.

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I. INTRODUCTION

The purpose of this paper is to report a robust method for reconstructing the detailed shape of a singular attractive potential from some of the bound-state spectral data that it generates. The general setting for the problem is the discrete spectrum of a Schrödinger Hamiltonian operator

$$H = -\Delta + vf(r), \quad r \equiv \|\mathbf{r}\|, \quad (1)$$

where $f(r)$ is the shape of an attractive central potential, and $v > 0$ is a coupling parameter. We shall assume that the potential is monotone non-decreasing and no more singular than the Coulomb potential $f(r) = -1/r$. The arguments we use apply generally to the problem in $d > 1$ spatial dimensions, but, for definiteness, we shall usually assume that $d = 3$. The operator inequality [1, 2]

$$-\Delta \geq \left(\frac{d/2 - 1}{r} \right)^2, \quad d \geq 3, \quad (2)$$

implies that a discrete spectrum exists for sufficiently large coupling $v > 0$. For $d = 3$, the Hamiltonian H is bounded below by

$$E \geq \min_{r>0} \left[\frac{1}{4r^2} + vf(r) \right], \quad (3)$$

and a simple trial function can be used to establish an upper bound. Thus we may assume, in particular, that the ground-state energy may be written as a function $E = F(v)$. An explicit example of the class of problems we consider is provided by the Hulthén potential whose shape is given by $f(r) = -1/(e^r - 1)$ and whose s-state ($\ell = 0$) eigenvalues E_n are given [3] exactly for $d = 3$ by the formula

$$E_n = F_n(v) = - \left(\frac{v - n^2}{2n} \right)^2, \quad v > n^2, \quad n = 1, 2, 3, \dots \quad (4)$$

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The problem discussed in the present paper may be stated as follows: given, for example, the curve $F_1(v)$, can we use this spectral data to reconstruct the potential shape $f(r)$? We call this ‘geometric spectral inversion’. It must be distinguished from ‘inverse scattering theory’ [4–12], and, in particular, from ‘the inverse problem in the coupling parameter’ [4]. In this latter problem, the energy eigenvalue E is fixed, and the data to be inverted comprises the set of all possible couplings leading to a radial eigenstate with this given energy, along with certain scattering data. In geometric spectral inversion, we simply use one spectral curve, say $F_1(v)$. Progress has been reported on this problem in a sequence of earlier papers [13–17]. From the point of view of problems in $d = 1$ dimension, we were at first concerned that for excited states, which often only exist for v sufficiently large, some essential pre-image data might be ‘missing’. However, the analytical inversion of the WKB approximation [15] showed that the WKB inversion process improves in quality as one goes to higher states, and is moreover asymptotically exact. Progress has been made on a related problem, namely on inverting spectral data of the form $E(\ell)$, where ℓ is the orbital angular momentum quantum number, for fixed coupling v ; this work by Grosse and Martin is described in Ref. [18].

We suggest two areas of application for the form of spectral inversion $F(v) \rightarrow f(r)$ which is the main topic of this paper. The spectrum generated by the outermost electron in a large atom is often estimated by use of a screened-Coulomb potential with parameters dependent on the atomic number Z . It is envisaged that atomic spectral data for a sequence of atomic numbers could be used to reconstruct an appropriate effective potential for the model. In another area, quantum field theory can be used to predict the dependence $E = F(v)$ of the energy of a two-body bound system on the coupling v . Geometric spectral inversion could then be used to construct from $F(v)$ a potential $f(r)$ that would reproduce the same spectrum in a quantum-mechanical model. The idea is that instead of fitting the parameters in an appropriate potential model, we instead develop an inversion method that allows us to reconstruct the potential shape directly from an eigenvalue curve.

In the present paper we study the inversion of spectral data arising from singular potentials. We develop a functional inversion algorithm based on envelope theory, a geometrical theory of energy functions such as $F_n(v)$. This was first introduced [19] in 1980 as a method for finding energy bounds for many-body problems, and has since led to a number of refinements and applications [20–24], including semirelativistic problems [25–29]. In sections II and III we first review enough of this theory to serve our present purpose and to make this paper essentially self-contained. In section IV we develop the inversion algorithm. We then test the algorithm on some concrete problems. In section V we show that the algorithm inverts spectral data arising from pure powers, or the log potential, exactly, in just two steps. In section VI we invert the Hulthén spectral data from Eq. (4). In section VII we apply the inversion algorithm to the spectral data generated by the family of potentials $f(r) = -a/r + bw(r)$, where $w(r) = r$, $w(r) = r^2$, and $w(r) = \ln(r)$. In these latter problems, for which analytic expressions for the spectral curves $F(v)$ are not available, we begin in each case with the potential $f(r)$, find $F(v)$ numerically (by shooting methods), and then apply the sequential inversion method presented in this paper to reconstruct $f(r)$ again from $F(v)$. The spectral *inversion* $F \rightarrow f$ is the principal concern of the present work. In section VIII we consider the ground state energy curve $F(v)$ for the problem $H = -\Delta + vg(r)/r$, where $g(0) < 0$, and $g'(r) \geq 0$. For this class of problems we prove that $F(v)$ determines $f(r) = g(r)/r$ uniquely.

II. EXACT REPRESENTATION OF SPECTRAL FUNCTIONS BY KINETIC POTENTIALS

The discrete spectra of operators such as $H = -\Delta + vf(r)$, which are bounded below, may be characterized variationally [30]. Thus, the ground-state energy may be written

$$F(v) = \inf_{\substack{\psi \in \mathcal{D}(H) \\ \|\psi\|=1}} (\psi, H\psi). \quad (5)$$

Since H depends on the coupling v , so therefore does the domain $\mathcal{D}(H)$. However, for the problems considered, either H has discrete eigenvalues, perhaps for v greater than some critical coupling v_1 , or the entire spectrum of H is discrete for $v > 0$. The kinetic potential $\bar{f}(s)$ associated with the potential shape $f(r)$ is defined (for the ground state) by a constrained minimization in which the mean kinetic energy $s = \langle -\Delta \rangle$ is kept constant:

$$\bar{f}(s) = \inf_{\substack{\psi \in \mathcal{D}(H) \\ \|\psi\|=1 \\ (\psi, -\Delta\psi)=s}} (\psi, f\psi). \quad (6)$$

The eigenvalue $F(v)$ of H is then recovered from $\bar{f}(s)$ by a final minimization over s :

$$F(v) = \min_{s \geq 0} [s + v\bar{f}(s)]. \quad (7)$$

The spectral function $F(v)$ is concave ($F''(v) < 0$); moreover, we have shown [13] that

$$F''(v)\bar{f}''(s) = -\frac{1}{v^3}. \quad (8)$$

Thus $F(v)$ and $\bar{f}(s)$ have opposite convexities and are related by the following Legendre transformations $\bar{f} \leftrightarrow F$ [31]:

$$\bar{f}(s) = F'(v), \quad s = F(v) - vF'(v), \quad (9)$$

$$1/v = -\bar{f}'(s), \quad F(v)/v = \bar{f}(s) - s\bar{f}'(s). \quad (10)$$

$F(v)$ is not necessarily monotone, but $\bar{f}(s)$ is monotone decreasing. Eq. (9) enables us also to work with the coupling as a minimization parameter. For this purpose we write the coupling as u and we have from Eq. (7)

$$F(v) = \min_{u>0} [F(u) - uF'(u) + vF'(u)]. \quad (11)$$

This is particularly useful in cases where $\bar{f}(s)$ is difficult to find explicitly.

By considering finite-dimensional linear spaces in $\mathcal{D}(H)$ we can extend these definitions and transformations [21, 24] to apply to the excited states. For example, in $d = 3$ dimensions, if D_n is an n -dimensional linear space of radial functions $\{\phi_i\}$ contained in $\mathcal{D}(H)$ and in the angular-momentum space labelled by Y_ℓ^m , then we have

$$E_{n\ell} = \inf_{D_n} \sup_{\substack{\psi \in D_n \\ \|\psi\|=1}} (\psi, H\psi). \quad (12)$$

We now scale the linear space D_n so that we can fix $\langle -\Delta \rangle = s$. We define a scaling operator $\hat{\sigma}$ by $(\hat{\sigma}\psi)(r) = \psi(\sigma r)$, $\sigma > 0$. Then, if we let

$$\hat{\sigma}D_n = \text{span}\{\hat{\sigma}\phi_i\}_{i=1}^n, \quad (13)$$

we may then define

$$\mathcal{D}_n = \bigcup_{\sigma>0} \hat{\sigma}D_n. \quad (14)$$

We note that this union of linear spaces is not itself a linear space. We may now define the excited-state kinetic potentials by

$$\bar{f}_{n\ell}(s) = \inf_{\mathcal{D}_n} \sup_{\substack{\psi \in \mathcal{D}_n \\ \|\psi\|=1 \\ (\psi, -\Delta\psi)=s}} (\psi, f\psi). \quad (15)$$

We shall not usually need to use this abstract definition since Eq. (9) enables us to generate kinetic potentials directly from known energy functions $F(v)$. For example, with the s-states for the Hulthén potential $f(r) = -1/(e^r - 1)$, we have from Eq. (4)

$$\bar{f}_n(s) = -\frac{1}{2} \left[\left[\frac{4s}{n^2} + 1 \right]^{\frac{1}{2}} - 1 \right], \quad n = 1, 2, 3, \dots \quad (16)$$

The point of these alternative expressions for the spectral curves will become clear when we discuss approximations in the next section. Another form of expression, useful for our present task, is obtained if we change the kinetic-energy parameter from s to r itself by inverting the (monotone) function $\bar{f}(s)$ to define the associated K -function by

$$K^{[f]}(r) = s = (\bar{f}^{-1} \circ f)(r). \quad (17)$$

Now the energy formula Eq. (7) becomes

$$F(v) = \min_{r>0} [K^{[f]}(r) + vf(r)]. \quad (18)$$

A sleight of hand may be perceived here since K depends on f . However, we do now have a relation that has F on one side and f on the other: our goal is to invert this expression, to effect $F \rightarrow f$. We shall do this in section (4) by using a sequence of approximate K -functions which do not depend on f .

Another class of soluble problems is the set of pure-power potentials the form of whose energy functions are determined by scaling arguments. We have [21]

$$f(r) = \text{sgn}(q) r^q \rightarrow F_{n\ell}^{(q)}(v) = E_{n\ell}(q) v^{\frac{2}{2+q}}, \quad q > -2, \quad q \neq 0, \quad (19)$$

where the unit-coupling eigenvalues $E_{n\ell}(q)$ are known in special cases, such as the Coulomb problem $E_{n\ell}(-1) = -1/(4(n+\ell)^2)$ and the harmonic oscillator $E_{n\ell}(2) = 4n + 2\ell - 1$, where $n = 1, 2, 3, \dots$ and $\ell = 0, 1, 2, \dots$. The corresponding kinetic potentials for this family become from Eqs. (9) and (19)

$$\bar{f}(s) = \frac{2}{q} \left| \frac{q E_{n\ell}(q)}{2+q} \right|^{\frac{q+2}{2}} s^{-\frac{q}{2}}. \quad (20)$$

By contrast, the K -functions are much simpler and are given by

$$K^{[q]}(r) = \frac{P_{n\ell}^2(q)}{r^2}, \quad (21)$$

where

$$P_{n\ell}(q) = |E_{n\ell}(q)|^{\frac{2+q}{2q}} \left[\frac{2}{2+q} \right]^{\frac{1}{q}} \left| \frac{q}{2+q} \right|^{\frac{1}{2}}, \quad q \neq 0. \quad (22)$$

For example

$$P_{n\ell}(-1) = n + \ell \quad \text{and} \quad P_{n\ell}(2) = 2n + \ell - \frac{1}{2}. \quad (23)$$

By defining $P_{n\ell}(0) = \lim_{q \rightarrow 0} P_{n\ell}(q)$, we not only make $P_{n\ell}(q)$ continuous at $q = 0$ but we also exactly accommodate the $\ln(r)$ potential [21]. It has been proved that the $P(q)$ functions are monotone increasing [22], and they appear to be concave. By contrast, the functions $E(q)$ are more complicated and have infinite slopes at $q = 0$. If we denote the eigenvalues of $-\Delta + \ln(r)$ by $E_{n\ell}^L$, we have by scaling

$$f(r) = \ln(r) \rightarrow F_{n\ell}(v) = -\frac{1}{2} v \ln(v/v_{n\ell}), \quad v_{n\ell} = \exp(2E_{n\ell}^L). \quad (24)$$

Meanwhile, the corresponding kinetic potential and K -function are given by

$$\bar{f}(s) = E_{n\ell}^L - \frac{1}{2} \ln(2es) \quad \text{and} \quad K^{[\ln]}(r) = \frac{P_{n\ell}^2(0)}{r^2}. \quad (25)$$

Numerical values for $P_{n\ell}(q)$ may be found for $d = 3$ in Ref. [32] and for more general $d > 1$ in Ref. [33].

The remaining task for this section is to note the scaling and invariance properties of $\bar{f}(s)$ and $K^{[f]}(r)$. We recall that, for a given eigenvalue, we recover the energy by the expressions

$$F(v) = \min_{s>0} [s + v\bar{f}(s)] = \min_{r>0} [K^{[f]}(r) + vf(r)].$$

It follows that if we scale and shift $f(r)$ to $A f(r/b) + B$, $a, b > 0$, then the new \bar{f} and K -functions are given by

$$\bar{f}(s) \rightarrow A \bar{f}(b^2 s) + B \quad \text{and} \quad K^{[f]}(r) \rightarrow \frac{1}{b^2} K^{[f]}(r/b). \quad (26)$$

The K -function has strong invariance since it must be employed with a changed $f(r)$ and the impacts of the parameters A and B are not overlooked. For pure powers and the log potential, the K -function is completely invariant with respect to this family of potential-shape transformations, including scale. We shall show in the next section that if $f(r) = g(h(r))$, and g is convex, then the approximation $K^{[f]} \approx K^{[h]}$ leads to energy lower bounds; it also removes f from K and suggests that inversion $F \rightarrow f$ might be possible via Eq. (18). When g is concave, we obtain upper bounds.

III. SMOOTH TRANSFORMATIONS AND ENVELOPE APPROXIMATIONS

In this section we consider potential shapes $f(r)$ that may be written as smooth transformations $f(r) = g(h(r))$ of a ‘basis potential’ $h(r)$. The idea is that we know the spectrum of $-\Delta + vh(r)$ and we try to use this to study the spectrum of $-\Delta + vf(r)$. When the transformation function g has definite convexity (g'' does not change sign), the kinetic-potential formalism immediately allows us to determine energy bounds. This is a consequence of Jensen’s inequality [34], which may be expressed in our context by the following:

$$\begin{aligned} g \text{ is convex } (g'' \geq 0) &\Rightarrow (\psi, g(h)\psi) \geq g((\psi, h\psi)), \\ g \text{ is concave } (g'' \leq 0) &\Rightarrow (\psi, g(h)\psi) \leq g((\psi, h\psi)). \end{aligned} \quad (27)$$

More specifically, we have for the kinetic potentials

$$g'' \geq 0 \Rightarrow \bar{f}(s) \geq g(\bar{h}(s)); \quad g'' \leq 0 \Rightarrow \bar{f}(s) \leq g(\bar{h}(s)). \quad (28)$$

We can summarize these results by writing $\bar{f}(s) \approx g(\bar{h}(s))$ and remembering that \approx is an inequality whenever g has definite convexity. The expression of these results in terms of K -functions is even simpler, for we have

$$K^{[f]} = \bar{f}^{-1} \circ f \approx (g \circ \bar{h})^{-1} \circ (g \circ h) = \bar{h}^{-1} \circ h = K^{[h]}. \quad (29)$$

Thus $K^{[f]} \approx K^{[h]}$ is the approximation we sought, that no longer depends on f . The corresponding energy bounds are provided by

$$E = F(v) \approx \min_{s>0} \{s + vg(\bar{h}(s))\} = \min_{r>0} \{K^{(h)}(r) + vf(r)\}. \quad (30)$$

Many examples and results derived from Eq. (30) have been discussed in earlier papers [19–24]. It remains here for us to describe another equivalent but geometrical approach which originally led, without Jensen’s inequality, to the term ‘envelope method’. This alternative is particularly useful when, as for the Dirac equation [35, 36], the kinetic-potential apparatus turns out to be complicated.

We study potentials of the form $f(r) = g(h(r))$ and we suppose that an eigenvalue of the operator $-\Delta + vh(r)$ is known and is given by $H(v)$. We now consider the ‘tangential potentials’ given by

$$f^{(t)}(r) = a(t)h(r) + b(t), \quad (31)$$

where the coefficients are

$$a(t) = g'(h(t)), \quad \text{and} \quad b(t) = g(h(t)) - h(t)g'(h(t)). \quad (32)$$

Thus the original potential $f(r)$ is the envelope of the family of tangential potentials $\{f^{(t)}(r)\}$. Let us suppose, for definiteness, that $g(h)$ is convex. Then each tangential potential is of the form $ah(r) + b$ lying below $f(r)$ and whose eigenvalues are known in terms of $H(v)$. Thus, the eigenvalue $F(v)$ of $-\Delta + vf(r)$ is bounded below by that of the ‘best’ lower tangential potential, the envelope of the family of lower energy curves. Explicitly, we have

$$F(v) \geq \max_{t>0} [H(a(t)v) + b(t)v]. \quad (33)$$

If we use the expressions for $a(t)$ and $b(t)$ given by Eq. (32), then we find that the critical point satisfies $H'(u) = h$, where $u = vg'(h)$. Meanwhile, the critical value is given by $H(u) - uH'(u) + vg(H'(u))$. But this is exactly what we obtain from the expressions $s = H(u) - uH'(u)$, $\bar{h}(s) = H'(u)$, and $\bar{f}(s) \approx g(\bar{h}(s))$, that is to say

$$F(v) \approx \min_{u>0} [H(u) - uH'(u) + vg(H'(u))]. \quad (34)$$

This corresponds to Eq. (11), with the envelope approximation for the kinetic potential.

IV. THE ENVELOPE INVERSION SEQUENCE

We suppose that an eigenvalue E of $H = -\Delta + vf(r)$ is known as function $E = F(v)$ of the coupling parameter $v > 0$. In some cases, such as the square well, the discrete eigenvalue may exist only for sufficiently large coupling, $v > v_1$. The kinetic potential $\bar{f}(s)$ may be obtained by inverting the Legendre transformation Eq. (9). Thus

$$F(v) = \min_{s>0} [s + v\bar{f}(s)] \rightarrow \bar{f}(s) = \max_{v>v_1} \left[\frac{F(v)}{v} - \frac{s}{v} \right]. \quad (35)$$

We shall also need to invert the relation Eq. (18) between $F^{[n]}$ and $K^{[n]}$ by means of

$$K(r) = \max_{v > v_1} [F(v) - v f(r)]. \quad (36)$$

We begin with a seed potential $f^{[0]}(r)$ from which we generate a sequence $\{f^{[n]}(r)\}_{n=0}^{\infty}$ of improving potential approximations. The idea behind this sequence is that we search for a transformation g so that $g(f^{[n]}(r))$ is close to $f(r)$ in the sense that the eigenvalue generated is close to $F(v)$. The envelope approximation is used at each stage. The best transformation $g^{[n]}$ at stage n is given by using the current potential approximation $f^{[n]}(r)$ as an envelope basis. We have:

$$\bar{f} = g^{[n]} \circ \bar{f}^{[n]} \Rightarrow g^{[n]} = \bar{f} \circ \bar{f}^{[n]-1}.$$

Thus

$$f^{[n+1]} = g^{[n]} \circ f^{[n]} = \bar{f} \circ K^{[n]}.$$

The resulting inversion algorithm may be summarized by the following:

inversion algorithm

$$f^{[n]}(r) \rightarrow F^{[n]}(v) \rightarrow K^{[n]}(r) = \max_{u > v_1} [F^{[n]}(u) - u f^{[n]}(r)], \quad (37)$$

$$f^{[n+1]}(r) = \max_{v > v_1} \left[\frac{F(v)}{v} - \frac{K^{[n]}(r)}{v} \right]. \quad (38)$$

The step $f^{[n]}(r) \rightarrow F^{[n]}(v)$ is effected by solving $(-\Delta + v f^{[n]})\psi = E\psi$ numerically for $E = F^{[n]}(v)$.

V. THE INVERSION OF SPECTRAL DATA FROM PURE POWERS AND THE LOG POTENTIAL

Suppose that the given spectral function $F(v)$ derives from a pure-power potential shape $f(r) = \text{sgn}(q)r^q$. Then according to Eq. (20) we know implicitly that the kinetic potential has the form $\bar{f}(s) = A(q) \text{sgn}(q) s^{-q/2}$. If we effect the inversion by starting, for example, with a Coulomb seed $f^{[0]}(r) = -1/r$, we have $K^{[0]}(r) = P(-1)^2/r^2$. It follows from the inversion algorithm that

$$f^{[1]}(r) = \bar{f}(K^{[0]}(r)) = \frac{A(q)}{(P(-1))^q} \text{sgn}(q) r^q.$$

Hence, by scaling Eq. (26), we find $K^{[1]}(r) = P(q)^2/r^2$, and, in one more step, we have

$$f^{[2]}(r) = \bar{f}(K^{[1]}(r)) = \text{sgn}(q) r^q = f(r).$$

Similarly, if $F(v)$ is generated by the log potential $f(r) = \ln(r)$, we have $F(v) = vF(1) - \frac{1}{2}v \ln(v)$. In this case, $\bar{f}(s) = F(1) - \frac{1}{2} \ln(2es)$. We again choose a Coulomb seed $f^{[0]}(r) = -1/r$, for which $K^{[0]}(r) = P(-1)^2/r^2$. It follows from the inversion algorithm that

$$\begin{aligned} f^{[1]}(r) = \bar{f}(K^{[0]}(r)) &= F(1) - \frac{1}{2} \ln(2eP(-1)^2/r^2) \\ &= F(1) - \frac{1}{2} \ln(2eP(-1)^2) + \ln(r). \end{aligned}$$

By scaling Eq. (26) we see that $K^{[1]}(r) = K^{[\ln]}(r) = P(0)^2/r^2$, and it follows that

$$f^{[2]}(r) = \bar{f}(K^{[1]}(r)) = \ln(r).$$

Any pure-power (or the log) seed would yield the same exact inversion in two steps for these cases.

VI. INVERSION OF HULTHÉN SPECTRAL FUNCTIONS

The Hulthén potential has shape $f(r) = -1/(e^r - 1)$ and s -state eigenvalues $F_n(v)$ given in Eq. (4). This potential has a Coulomb-like singularity at the origin as evidenced by the Coulomb-like behaviour $F_n(v) \sim -c v^2$ of the spectral curves for large v . We therefore use a Coulomb seed $f^{[0]}(r) = -1/r$ to begin the inversion of $F(v) = F_1(v)$. As before, we have from this seed that $K^{[0]}(r) = P(-1)^2/r^2$. The first inversion step can be made analytically. By using $\bar{f}(s)$ from Eq. (16) with $n = 1$ we obtain

$$f^{[1]}(r) = \bar{f}(K^{[0]}(r)) = -\frac{1}{2} \left[\left[\frac{4}{r^2} + 1 \right]^{\frac{1}{2}} - 1 \right]. \quad (39)$$

This step is shown in Fig. (1) as the curve clearly between the seed and the ‘goal’. The iteration is repeated twice more numerically and the graph shows $f^{[3]}(r)$, which almost coincides with the goal $f(r)$. We have found similar convergence when inverting excited-state spectral curves $F_n(v)$ for $n > 1$ by the same algorithm. The convergence is better in these cases if the seed K -function $K^{[0]}(r) = (P_{n\ell}(-1)/r)^2$ corresponds to the same radial excitation $P_{n\ell}(-1) = n + \ell = n$ as that of the energy curve that is being inverted; with this choice, the first iteration $f^{[1]}(r)$ is *exactly* given by Eq. (39) for all $n \geq 1$.

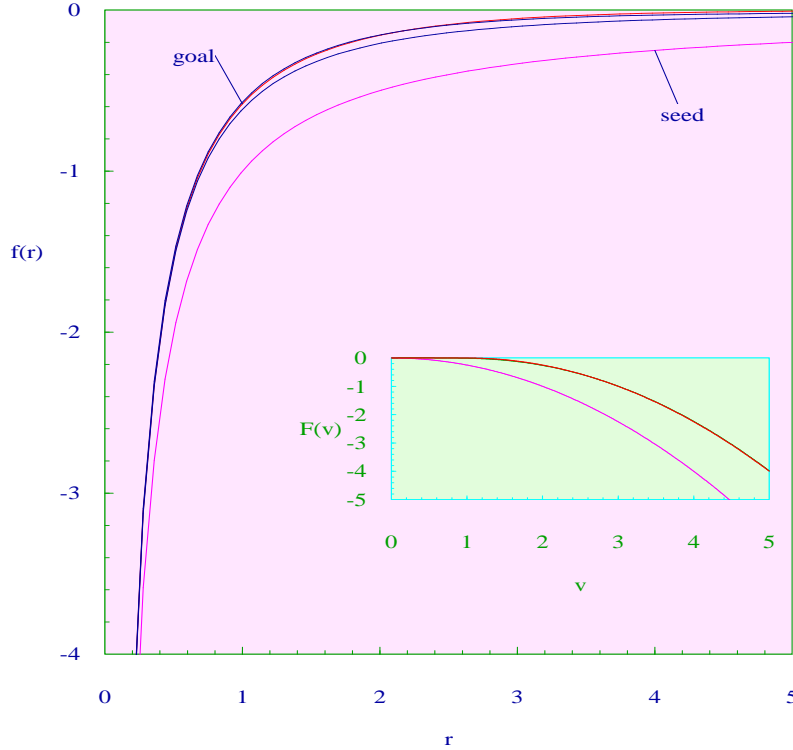


FIG. 1: The inversion of Hulthén spectral data $F(v) = -(v-1)^2/4$, $v \geq 1$, shown as the upper inset curve; the lower inset curve is the Coulomb spectral function $-v^2/4$. In the main graphs the Coulomb seed $f^{[0]}(r) = -1/r$ is used to start the inversion iteration sequence. The diagram also shows the first iteration $f^{[1]}(r)$ and the third iteration $f^{[3]}(r)$, which almost coincides with the Hulthén goal $f(r) = -1/(e^r - 1)$.

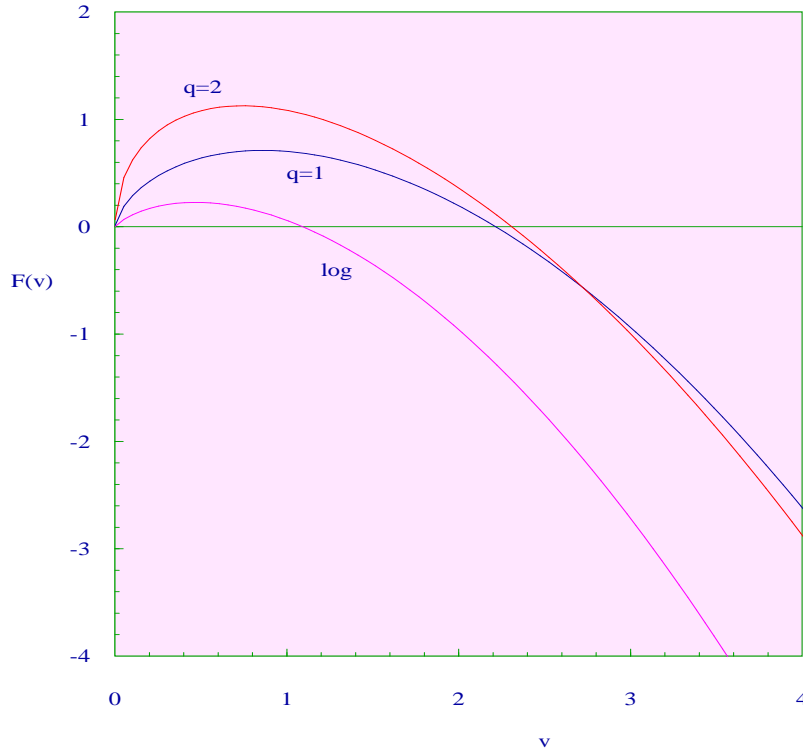


FIG. 2: The ground-state eigenvalue curves $F(v)$ for the operator $H = -\Delta + v(-1/r + \frac{1}{2}w(r))$, where $w(r)$ is respectively r , r^2 , and $\ln(r)$. The inversion of these spectral curves are shown respectively in Figs. (3 - 5).

VII. INVERSION OF SPECTRAL DATA FROM POTENTIALS OF THE FORM $f(r) = -a/r + bw(r)$, WHERE $w(r) = \text{sgn}(q)r^q$ OR $\ln(r)$.

We now consider three examples of spectral data arising from singular potentials of the form

$$f(r) = -\frac{a}{r} + bw(r), \text{ where } w(r) = r, r^2, \ln(r). \quad (40)$$

Graphs of the corresponding ground-state energy functions $F(v)$ for $a = 1$ and $b = \frac{1}{2}$ are shown in Fig.(2). The inversion algorithm of section (4) has been applied to each of these spectral curves and the results are shown in Figs. (3-5). In each case the seed potential was the Coulomb potential $f^{[0]}(r) = -1/r$. The curve lying above the goal is the first iteration $f^{[1]}(r)$; the third iteration is also shown and is in each case very close to the goal of the example, namely $f(r)$ itself.

VIII. UNIQUENESS

An important issue concerning the inversion $F \rightarrow f$ is whether there is more than one inverse f for a given F . We tackled this question earlier, in Ref. [14] §6, for bounded symmetric potentials in $d = 1$ dimension that were monotone non-decreasing on the half-line $x > 0$: under these conditions, the inverse was shown to be unique. It is straightforward to prove a similar theorem for bounded potentials in three dimensions. However, a new theorem is needed for singular potentials. We suppose in $d = 3$ dimensions that the potential shape $f(r)$ is attractive, spherically symmetric, and Coulombic for small r ; more specifically, we shall assume that $f(r)$ can be written in the form

$$f(r) = \frac{g(r)}{r}, \quad \text{where } g(0) < 0, g'(r) \geq 0, \quad (41)$$

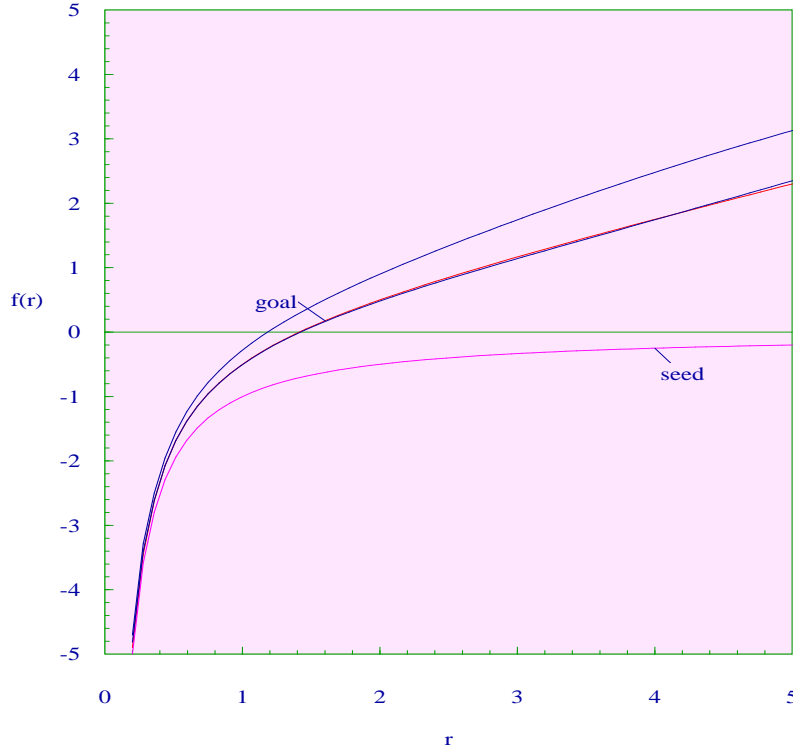


FIG. 3: The inversion of the spectral data shown in Fig. (2) for the Coulomb-plus-linear potential $f(r) = -1/r + \frac{1}{2}r$. The diagram shows the seed $f^{[0]}(r) = -1/r$, the first iteration $f^{[1]}(r)$, and the third iteration $f^{[3]}(r)$, which almost coincides with the goal, the exact potential $f(r)$.

and $g(r)$ is not constant. Examples of this class of singular potential shapes are Yukawa $g(r) = -e^{-ar}$, Hulthén $g(r) = -r/(e^{ar} - 1)$, and linear-plus-Coulomb $g(r) = -a + br^2$, with $a, b > 0$. We consider the ground state $\psi(r, v)$ which we suppose to be a normalized radial function so that

$$\int_0^\infty \psi^2(r, v) r^2 dr = 1. \quad (42)$$

With these assumptions, we shall prove the following

Theorem 1 *The potential shape $f(r)$ in $H = -\Delta + vf(r)$ is uniquely determined by the ground-state energy function $E = F(v)$.*

Proof

For this singular class of potentials it is helpful to consider an additional probability density on $[0, \infty)$ of the form $c\psi^2(r, v)r$ and to define the integrals

$$q(a, v) = \int_0^a \psi^2(r, v) r dr \quad \text{and} \quad I(v) = \int_0^\infty \psi^2(r, v) r dr. \quad (43)$$

In this sense, $Q(a, v) = q(a, v)/I(v)$ is the probability mass on $[0, a]$. Our first task is to establish a concentration lemma to the effect that, for each fixed a , this probability $Q(a, v) \rightarrow 1$ as v increases without limit. From Eq. (9) we have

$$F'(v) = \int_0^\infty \psi^2(r, v) r^2 f(r) dr = \int_0^\infty \psi^2(r, v) r g(r) dr \geq I(v)g(0) \quad (44)$$

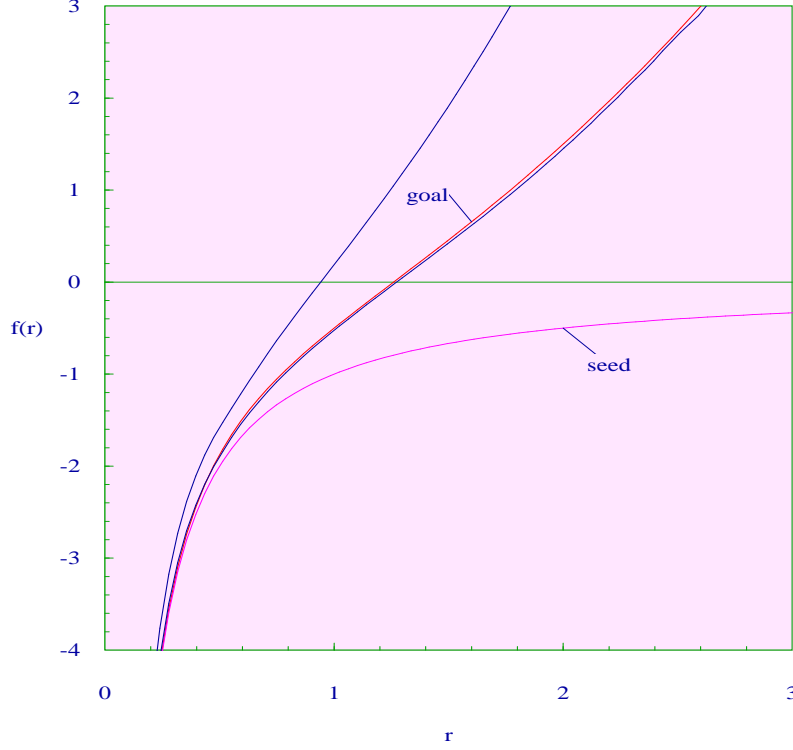


FIG. 4: The inversion of the spectral data shown in Fig. (2) for the Coulomb-plus-oscillator potential $f(r) = -1/r + \frac{1}{2}r^2$. The diagram shows the seed $f^{[0]}(r) = -1/r$, the first iteration $f^{[1]}(r)$, and the third iteration $f^{[3]}(r)$, which almost coincides with the goal, the exact potential $f(r)$.

and

$$F'(v) = \int_0^a \psi^2(r, v) r g(r) dr + \int_a^\infty \psi^2(r, v) r g(r) dr \geq q(a, v) g(0) + (I(v) - q(a, v)) g(a). \quad (45)$$

Thus we find for each a such that $g(a) > g(0)$,

$$1 \geq Q(a, v) = \frac{q(a, v)}{I(v)} \geq \frac{g(a) - F'(v)/I(v)}{g(a) - g(0)}. \quad (46)$$

For large v the potential shape is spectrally dominated by the Coulomb term $vf(r) \sim vg(0)/r$. The corresponding wave function, eigenvalue, and $I(v)$ are given asymptotically by

$$\psi(r, v) \sim ce^{vg(0)r/2}, \quad F(v) \sim -\frac{(vg(0))^2}{4}, \quad \text{and} \quad I(v) \sim \frac{|vg(0)|}{2}. \quad (47)$$

It follows that $F'(v)/I(v) \sim g(0)$. By using these asymptotic expressions in Eq. (43) and Eq. (44) we arrive at the limit

$$\lim_{v \rightarrow \infty} \left(\frac{F'(v)}{I(v)} \right) = g(0). \quad (48)$$

Thus, for each fixed a such that $g(a) > g(0)$, we have the **radial concentration lemma**

$$1 \geq Q(a, v) \geq \frac{g(a) - F'(v)/I(v)}{g(a) - g(0)} \rightarrow 1. \quad (49)$$

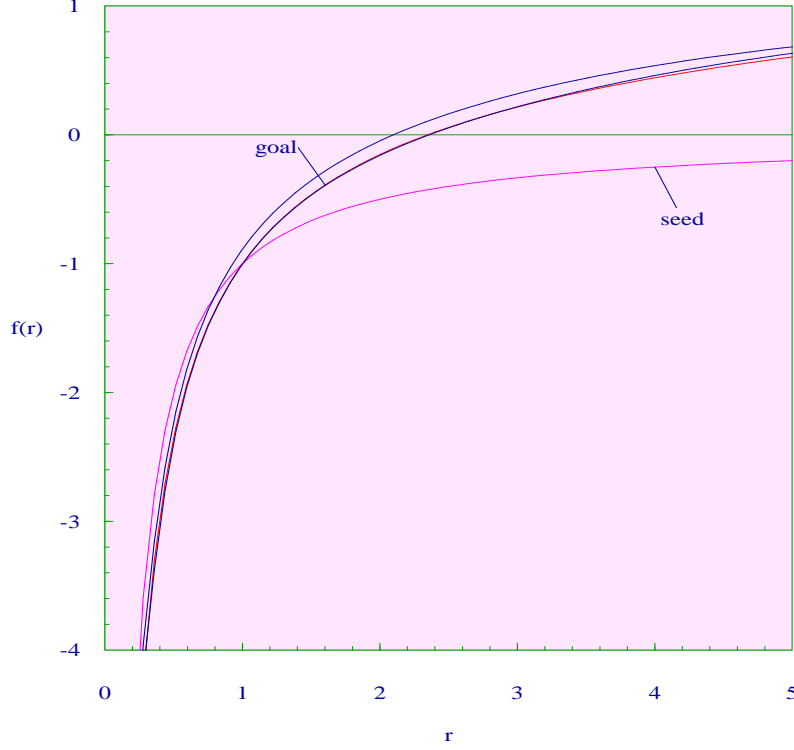


FIG. 5: The inversion of the spectral data shown in Fig. (2) for the Coulomb-plus-log potential $f(r) = -1/r + \frac{1}{2} \ln(r)$. The diagram shows the seed $f^{[0]}(r) = -1/r$, the first iteration $f^{[1]}(r)$, and the third iteration $f^{[3]}(r)$, which almost coincides with the goal, the exact potential $f(r)$.

Now let us suppose that the two potential shapes $g(r)/r$ and $(g(r) + \gamma(r))/r$ both have the same ground-state energy function $F(v)$. We shall prove that $\gamma = 0$. By considering large v we see from Eq. (47) that $\gamma(0) = 0$. We consider the two Hamiltonians $H = -\Delta + v g(r)/r$ and $H_1 = -\Delta + v (g(r) + \gamma(r))/r$ with respective lowest normalized radial eigenstates $\psi(r, v)$ and $\phi(r, v)$, $J(v) = \int_0^\infty \phi^2(r, v) r dr$, and the common eigenvalue curve is $F(v)$. From the equalities

$$(\psi, H\psi) = F(v) = (\phi, H_1\phi) \quad (50)$$

and the variational inequalities

$$(\psi, H_1\psi) \geq F(v) \leq (\phi, H\phi) \quad (51)$$

we deduce the complimentary inequalities

$$(\phi, \gamma(r)/r \phi) = \int_0^\infty \phi^2(r, v) \gamma(r) r dr \leq 0 \leq \int_0^\infty \psi^2(r, v) \gamma(r) r dr = (\psi, \gamma(r)/r \psi). \quad (52)$$

Thus

$$\frac{1}{J(v)} \int_0^\infty \phi^2(r, v) \gamma(r) r dr \leq 0 \leq \frac{1}{I(v)} \int_0^\infty \psi^2(r, v) \gamma(r) r dr. \quad (53)$$

By a sweeping process starting at $r = 0$ we now show that Eq. (53) implies that $\gamma \equiv 0$. We know that $\gamma(0) = 0$. Clearly, if $\gamma(r)$ does not change sign, then it must vanish identically. Let us suppose that $\gamma(r)$ first changes sign at $r = a$; more specifically (and without loss of generality), we suppose $\gamma(r) \geq 0$ for $r \in (0, a)$, and that $\gamma(a) = 0$. We

first note that if $g(a) = g(0)$, $g(r)$ would be constant on $[0, a]$ and $\gamma(r)$ would have to vanish on $[0, a]$ in order for $(g(r) + \gamma(r))/r$ to remain in the same potential class. Thus we understand $r = a$ to be the first point where $\gamma(r)$ is zero, after it has been positive. We now increase v so that both of the following inequalities are satisfied

$$\frac{F'(v)}{I(v)} < g(a), \quad \frac{F'(v)}{J(v)} < g(a) + \gamma(a) = g(a). \quad (54)$$

In view of the radial concentration lemma, further increase in v will force both integrals in Eq. (53) to be positive. This cannot be unless $\gamma \equiv 0$. This establishes Theorem 1. \square

IX. CONCLUSION

We are presented with a spectral curve, $F(v)$, which shows how a discrete eigenvalue of the Hamiltonian $H = -\Delta + vf(r)$ depends on the coupling parameter $v > 0$. From this data, we reconstruct the underlying potential shape $f(r)$. This ‘geometric spectral inversion’ is effected by a functional sequence in which the unknown potential shape $f(r)$ is first regarded as a smooth transformation $g(f^{[0]}(r))$ of a seed potential $f^{[0]}(r)$. The paper focuses on problems that involve singular potentials for which the Coulomb seed $f^{[0]}(r) = -1/r$ is very effective. The method of potential envelopes is used to generate a sequence of approximations $\{f^{[n]}(r)\}_{n=0}^{\infty}$ for which the corresponding transformations gradually approach the identity. At this stage of the investigation we offer an explicit heuristic inversion algorithm rather than an abstract convergence theorem. However, for the class of attractive central potentials with shapes $f(r) = g(r)/r$, with $g(0) < 0$ and $g'(r) \geq 0$, we prove that the ground-state energy curve $F(v)$ determines $f(r)$ uniquely.

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